AFRL-RW-EG-TP-2011-023

Benchtop Energetics Progress

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AIR FORCE RESEARCH LABORATORY, MUNITIONS DIRECTORATE

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14. ABSTRACT

We have constructed an apparatus for investigating the reactive chemical dynamics of mg-scale energetic materials samples. We seek to advance the understanding of the reaction kinetics of energetic materials, and of the chemical influences on energetic materials sensitivity. We employ direct laser irradiation, and indirect laser-driven shock, techniques to initiate thin-film explosive samples contained in a high-vacuum chamber. Expansion of the reacting flow into vacuum quenches the chemistry and preserves reaction intermediates for interrogation *via* time-of-flight mass spectrometry (TOFMS). By rastering the sample coupon through the fixed laser beam focus, we generate hundreds of repetitive energetic events in a few minutes.

A detonation wave passing through an organic explosive, such as pentaerythritol tetranitrate (PETN, $C_5H_4N_4O_{12}$), is remarkably efficient in converting the solid explosive into final thermodynamically-stable gaseous products (*e.g.* N_2, CO_2, H_2O…). Termination of a detonation at an explosive-to-vacuum interface produces an expanding pulse of hyperthermal molecular species, with leading-edge velocities ~ 10 km/s. In contrast, deflagration (subsonic combustion) of PETN in vacuum produces mostly reaction intermediates, such as NO and NO_2, with much slower molecular velocities; consistent with expansion-quenched thermal decomposition of PETN. We propose to exploit these differences in product chemical identities and molecular species velocities to provide a chemically-based diagnostic for distinguishing between detonation and deflagration events.

In this talk we also report recent progress towards the quantitative detection of hyperthermal neutral species produced by direct laser ablation of aluminum metal and of organic energetic materials, as a step towards demonstrating the ability to discriminate slow reaction intermediates from fast thermodynamically-stable final products.

15. SUBJECT TERMS
Detonation, deflagration, TOFMS, laser ablation

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Benchtop Energetics Progress

17th Biennial International Conference
American Physical Society Topical Group
Shock Compression of Condensed Matter
27 June 2011

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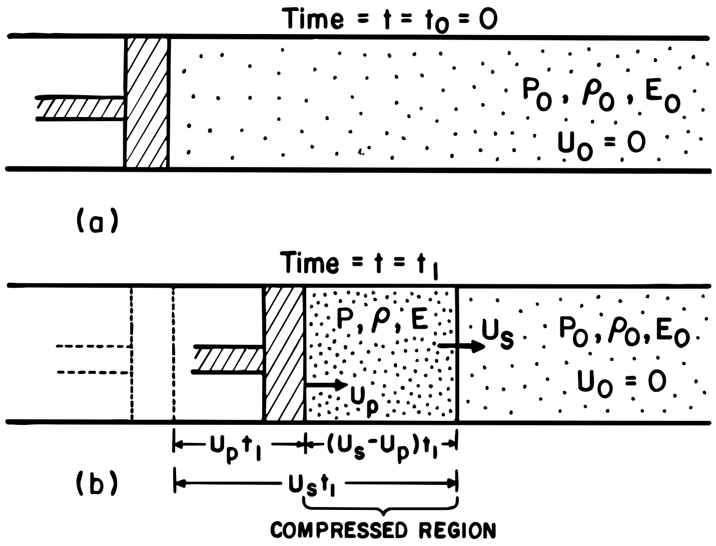
Monday 12:15PM C2.00005
Benchtop Energetics:
Detection of Hyperthermal Species

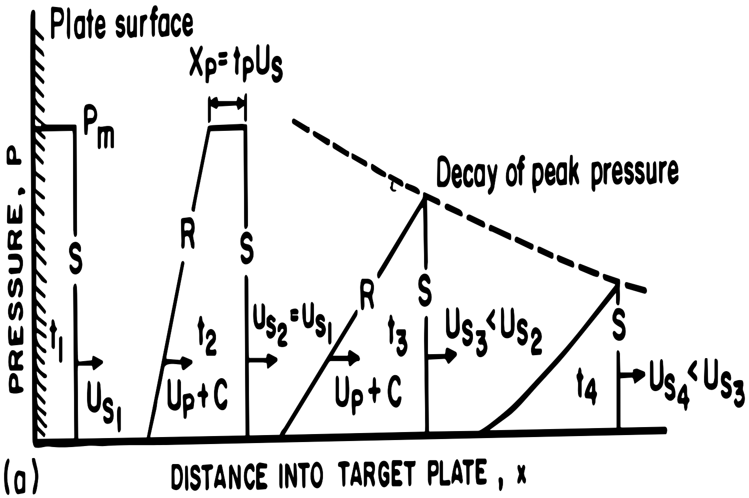
Dr. Christopher D. Molek
NRC Postdoc
University of Florida REEF
AFRL/RWME

Outline

- **Introduction**
  - Shock Wave and Detonation Cartoons
  - Hyperthermal Species from Explosions *In Vacuo*
- **1st Generation Experiment**
  - Laser Driven Flyers and Time-Of-Flight Mass Spectrometry (TOFMS)
  - PETN Deflagration Quenched by Vacuum Expansion
  - No Hyperthermal Species Detected
- **2nd Generation Experiment**
  - Apparatus Modifications – Differential Pumping
  - SIMION Simulations of Ion Trajectories within TOFMS
  - Detection of Fast Aluminum Atoms from Laser Ablation
  - Nitrocellulose Laser Initiation Preliminary Results
- **Conclusions & Future Directions**

Shock Waves





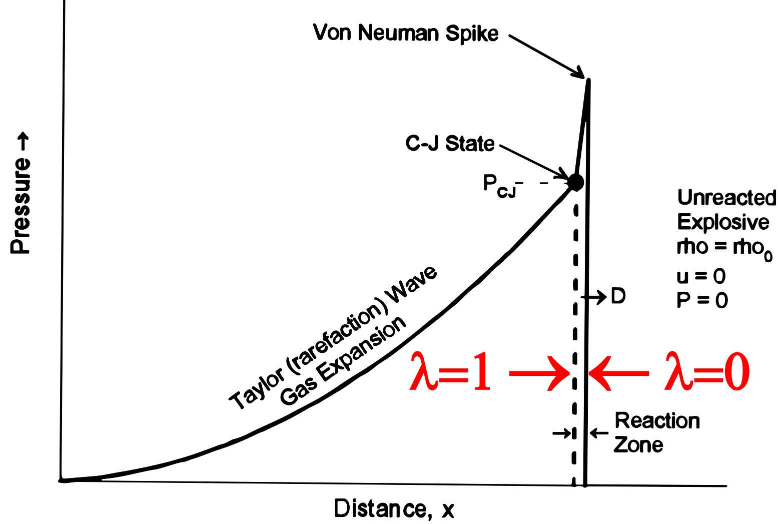
Shock Wave: a discontinuity in a material's properties (pressure, density, internal energy, etc.) propagating faster than the speed of sound in the undisturbed material.

Unsupported shock waves eventually decay into sound waves.

M.A. Meyers, Dynamic Behavior Of Materials (Wiley-Interscience, New York, 1994).

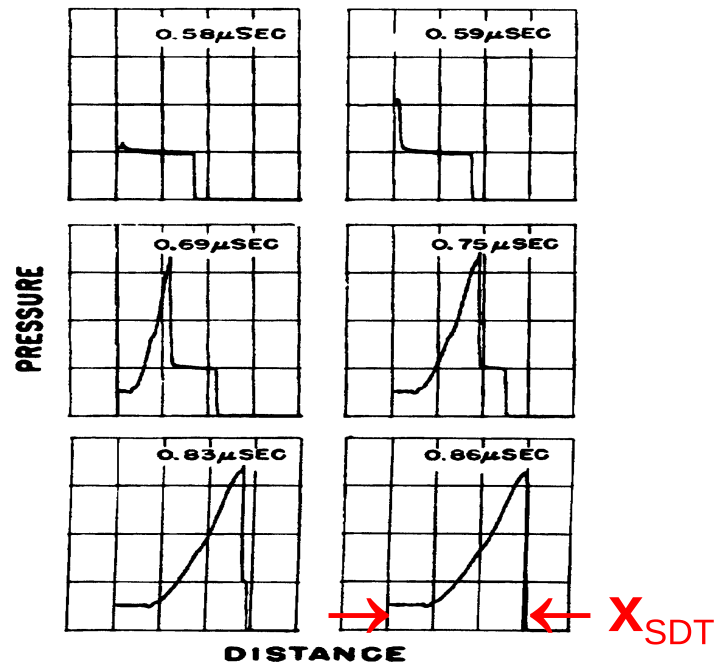
Detonation Waves

@ steady state:



Detonation Wave: a shock wave supported by a rapid exothermic chemical reaction.

P.W. Cooper, Explosives Engineering (Wiley-VCH, New York, 1996).



Initiation of nitromethane by 90 kbar shock (SIN simulation).

C.L. Mader, Numerical Modeling of Explosives and Propellants (CRC Press, Boca Raton, 1998).

Monday 11:30AM C2.00002, A Hydrocode Study of Explosive Shock Ignition, G. BUTLER & Y. HORIE, AFRL/RWME.

Hypervelocity Species

JOURNAL OF APPLIED PHYSICS VOLUME 42, NUMBER 2 FEBRUARY 1971

Explosive Gas Blast: The Expansion of Detonation Products in Vacuum

THOMAS J. AHRENS
Seismological Laboratory, California Institute of Technology, Pasadena, California 91109
AND
CHARLES F. ALLEN
Stanford Research Institute, Menlo Park, California 94205
AND
ROBERT L. KOVACH
Department of Geophysics, Stanford University, Stanford, California 94305

(Received 18 May 1970; in final form 4 September 1970)

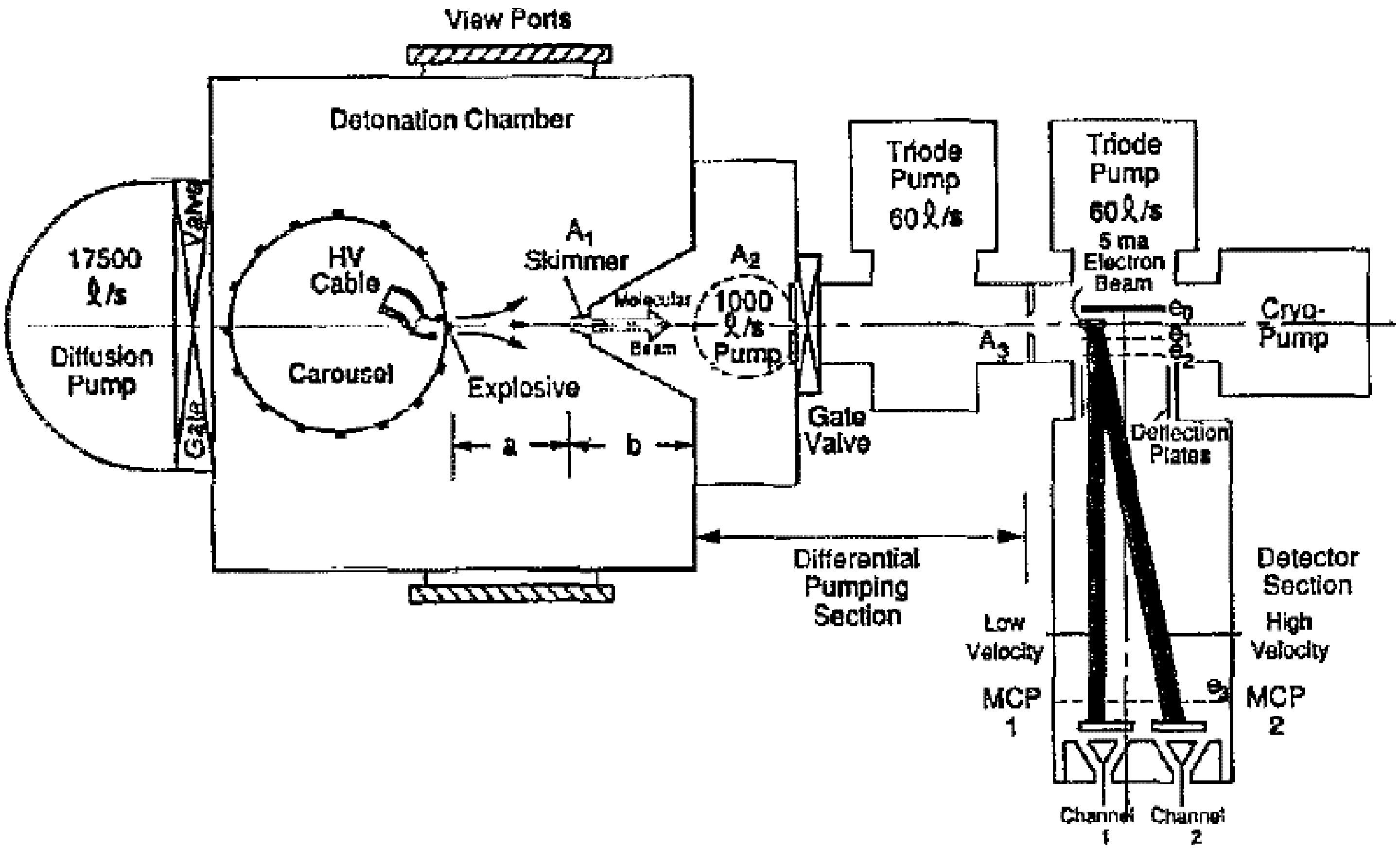
A series of 0.2- to 3-gm HNS charges were detonated in vacuums of 10^{-3} to 10^{-5} Torr. The resultant freely expanding, detonation product, gas blast achieves terminal velocities of 8 to 12 km/sec within 3 to 5 μsec after the detonation wave arrives at the free surface. Measured pressure profiles display rise times to maximum stagnation ("reflected shock") pressure varying from ~30 μsec, 20-cm away from a 2.6-gm charge, to ~185 μsec, 127-cm away from 0.2-gm charge at 10^{-5} Torr. Rise times were generally shorter at 10^{-3} and 10^{-4} Torr; the 10^{-5} Torr values agree with numerical calculations. Using cube root scaling of charge mass, the observed peak reflected pressure as a function of range may be represented by

$$p = 6.5\times10^{5}\ (\text{bar})\ r'^{-3.5},$$

where r' the ratio of the range to the equivalent charge radius.

Expect fast, thermodynamically stable products from detonations.

Benchmark Experiments



N.C. Blais, H.A. Fry, N.R. Greiner, Rev. Sci. Instrum. **64**, 174 (1993).

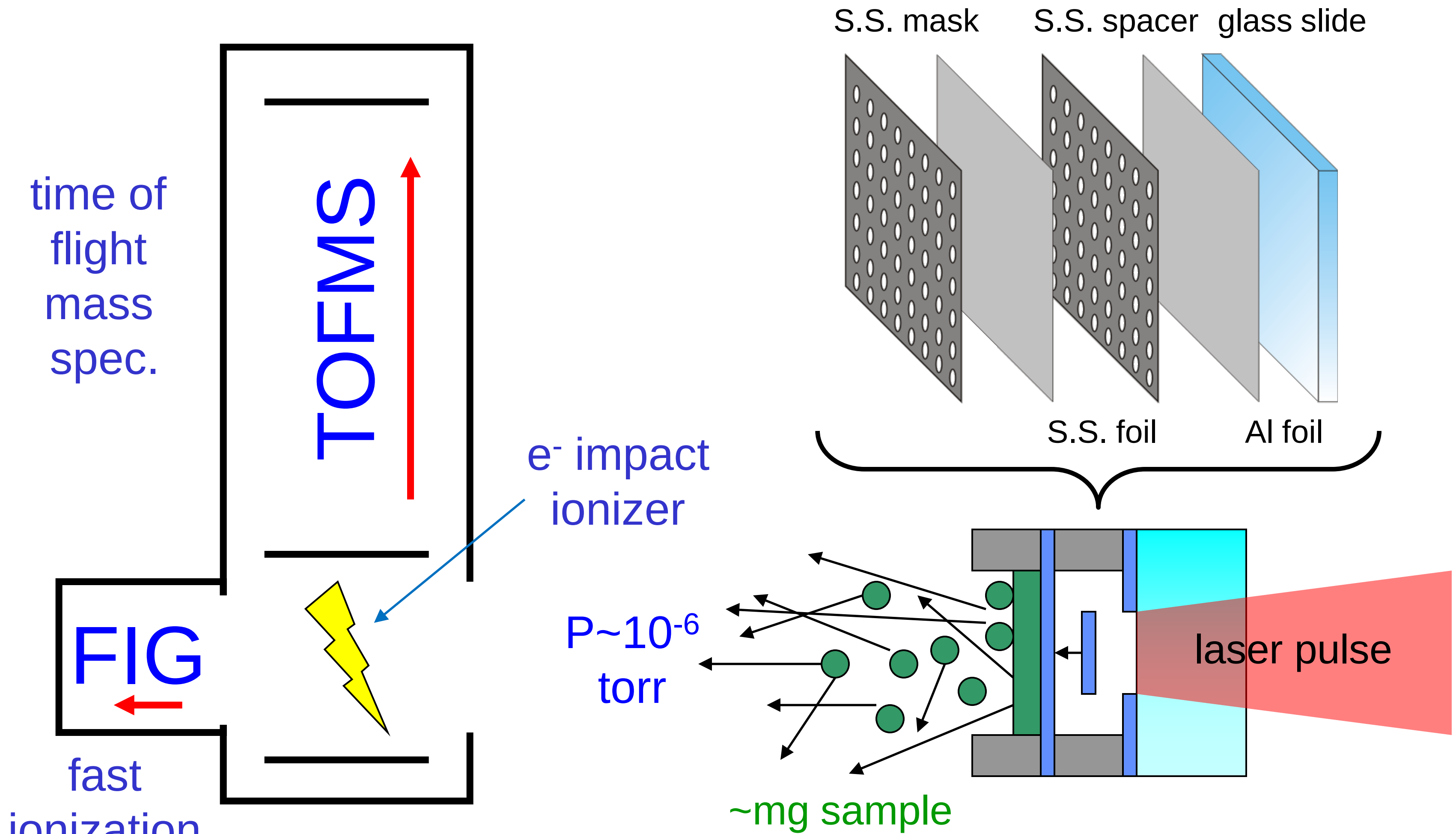
Observed both fast and slow species, intermediates and products.

Our Approach & Challenges

Approach:
- Laser-driven shock ignition/initiation of ~ mg samples
- Vary sample thickness over putative characteristic length scales: reaction zone, run to detonation...
- Spectroscopic and mass spectrometric diagnostics
- Statistically meaningful number of measurements

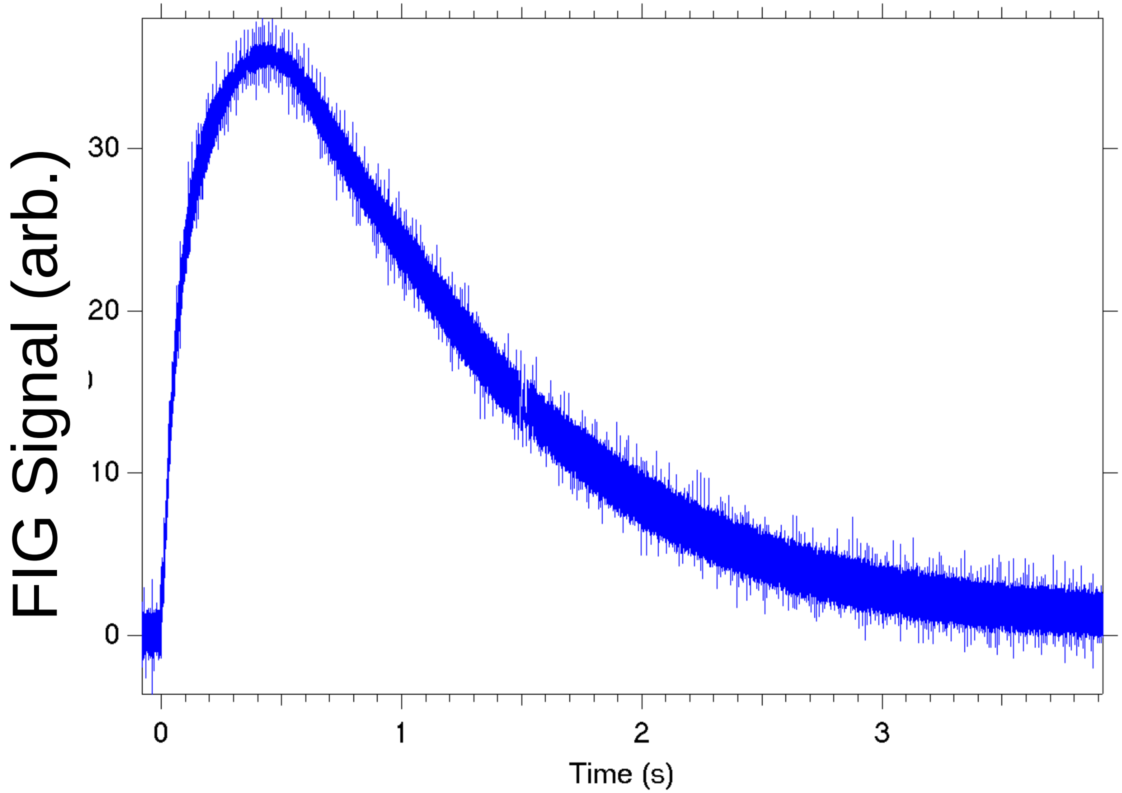
Challenges:
- Controlled, quantifiable ignition/initiation conditions
  - reproducible, plentiful laser-driven flyers
  - sample preparation & characterization
- Observation/interpretation of mass spectrometric data
  - qualitative: fragments/products, slow/fast velocities
  - quantitative species assignments

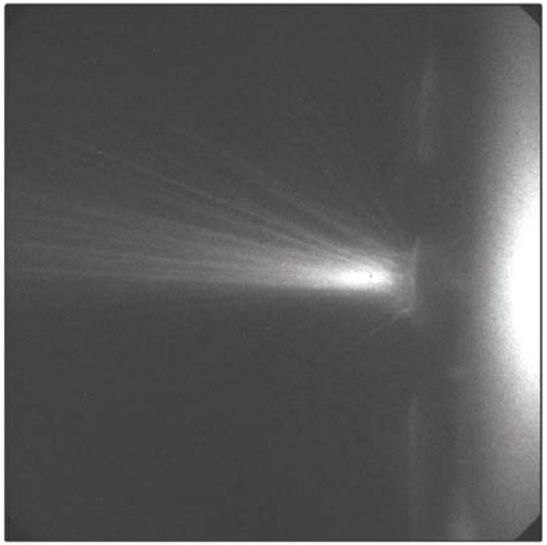
1st Generation Expt. Schematic



c.f.: S.J. Buelow, *et al*., APS SCCM **706**, 1377 (2004).
I.Y.S. Lee, *et al*., J. Appl. Phys. **75**, 4975 (1994).

Slow Gas Production by PETN



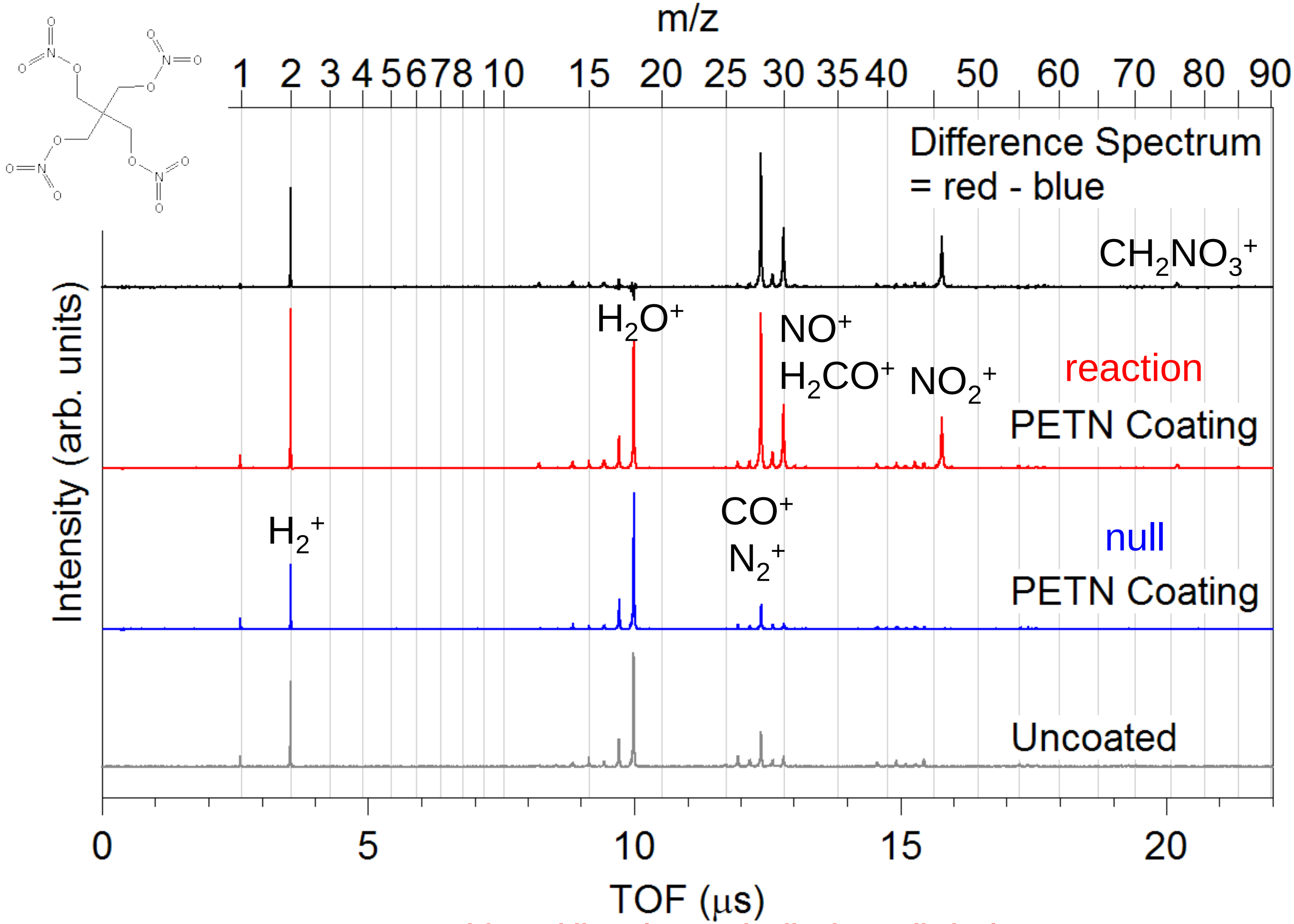


Deflagrating PETN particles; v ~ 1 m/s

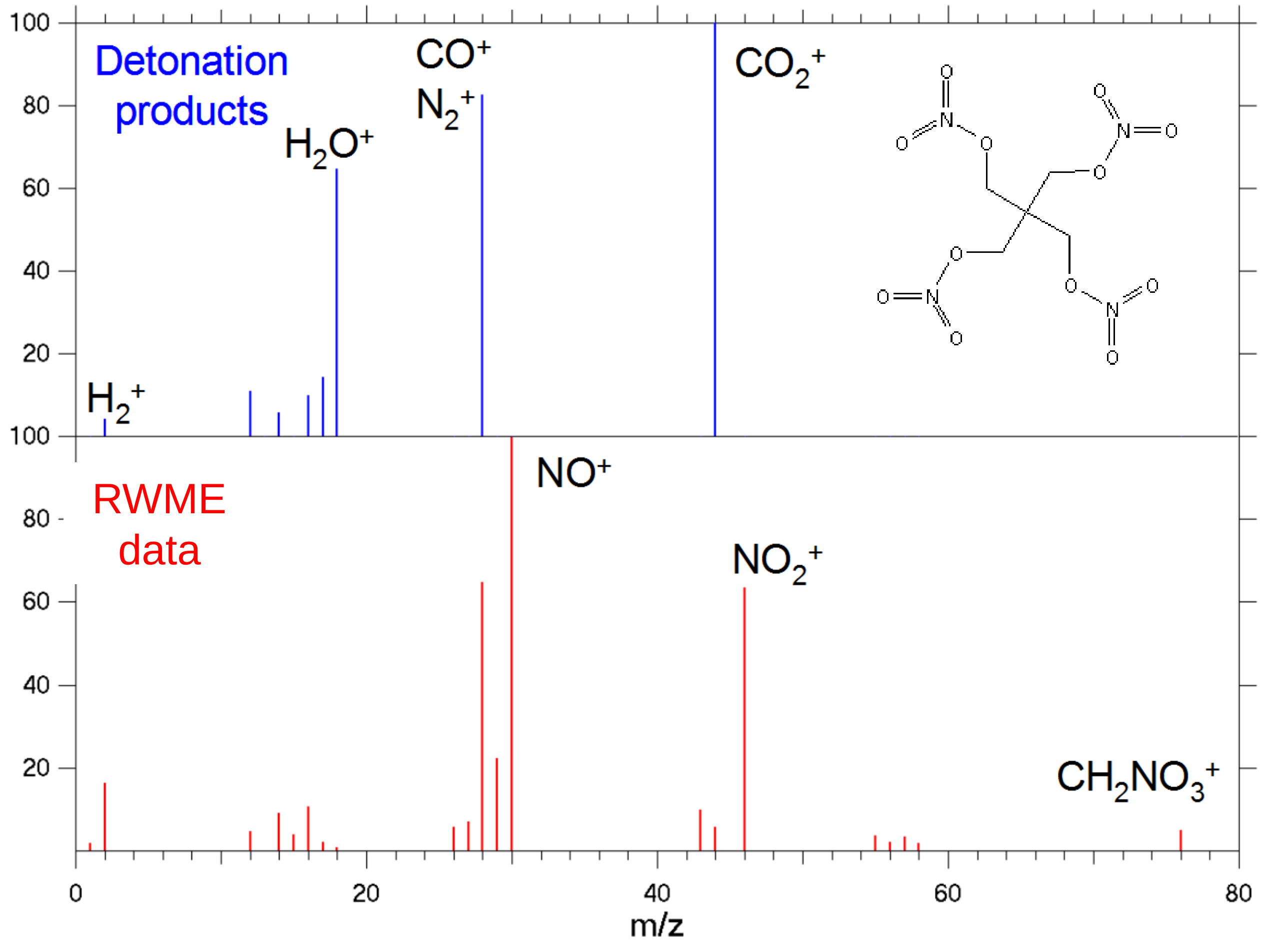
Expected: direct observation of products traveling line-of-sight to TOFMS.
N.C. Blais, H.A. Fry, N.R. Greiner, Rev. Sci. Instrum. 64, 174 (1993).

Actual: products endure multiple collisions with vacuum chamber walls
$\Rightarrow$ strong detection bias towards chemically stable, volatile species.

Mass Spectrometry of PETN



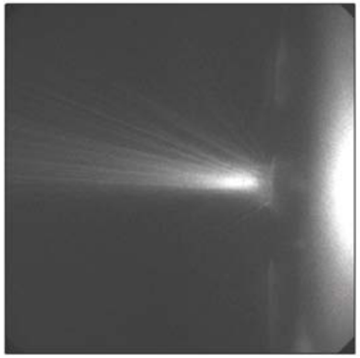
PETN Reaction Chemistry



Products (moles/mole PETN):

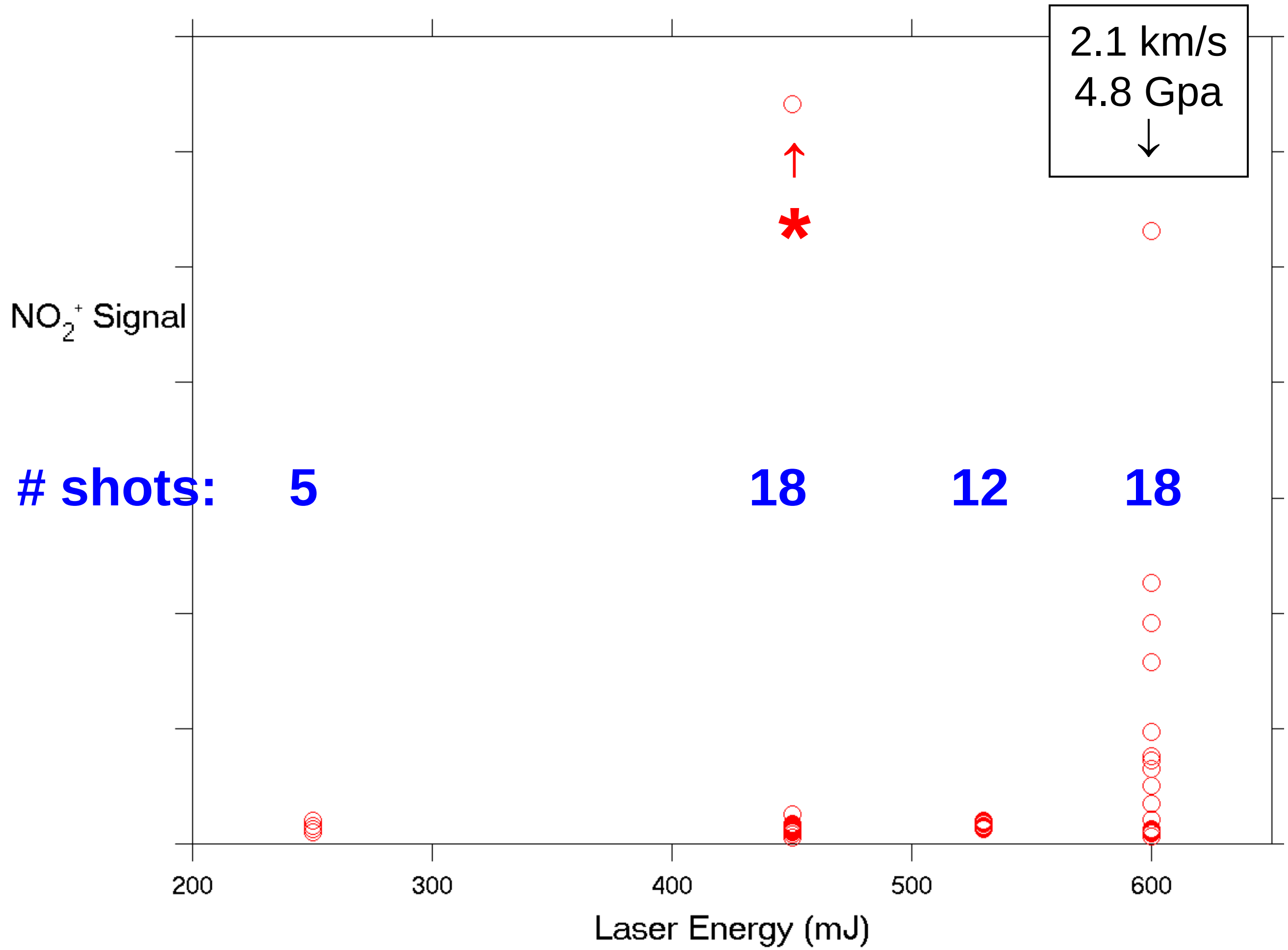
CO_2	3.50±0.04
CO	1.56±0.08
N_2	2.00±0.04
H_2	0.51±0.04
H_2O	3.45±0.04
NH_3	<0.0002
CH_4	<0.0002

D. Ornellas, et al., Rev. Sci. Instrum. **37**, 907 (1966).



Deflagrating PETN; thermal decomposition quenched by expansion into vacuum.

PETN Ignition Threshold (Almost*)



← flyer velocity
←peak pressure (estimated)

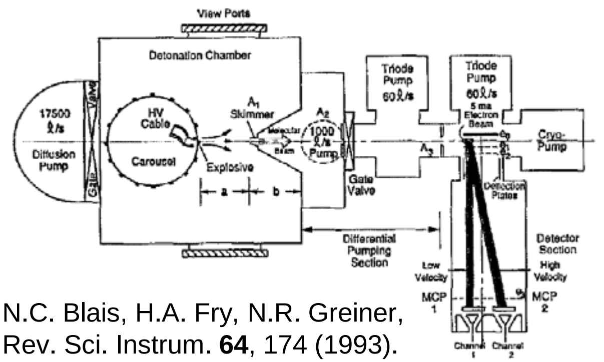
Threshold for laser-flyer initiation of <u>detonation</u> in macroscopic PETN samples is 7.1 ± 0.2 GPa.

[G. Zhuowei, et al., J. Appl. Phys. **96**, 344 (2004)].

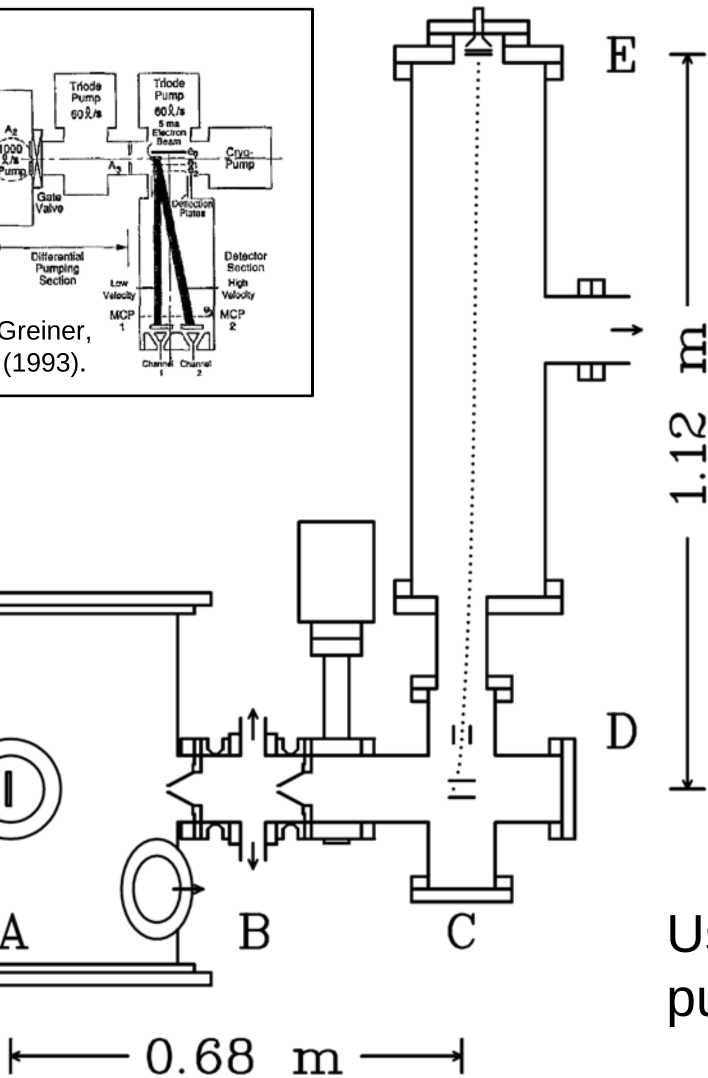
1st Generation Expt. Summary

- Demonstrated working laser-flyer initiation + mass spectrometric product characterization apparatus.
- Detected onset of chemical reactions in PETN -- at a “reasonable” threshold shock pressure.
- Observed reaction products consistent with thermal decomposition quenched by vacuum expansion.
- However, failed to detect either hyperthermal species from PETN, *OR* fast Al atoms in aluminum laser ablation experiments.

Add Differential Pumping Region



N.C. Blais, H.A. Fry, N.R. Greiner, Rev. Sci. Instrum. **64**, 174 (1993).



A – Main Chamber

B – Differential Pumping

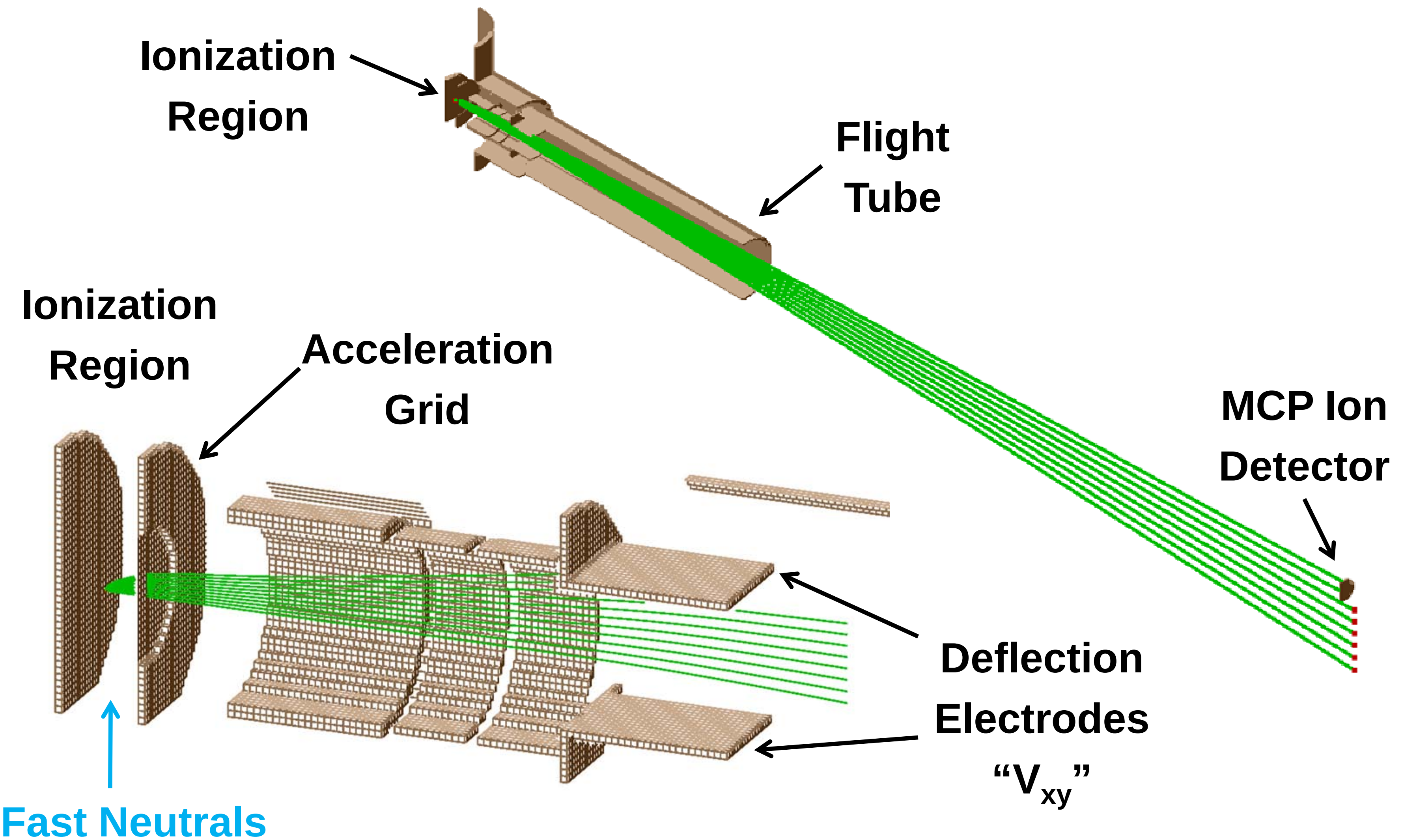
C – Ionization Region

D – Deflection Region

E – MCP Ion Detector

Use skimmers and differential pumping to form molecular beam.

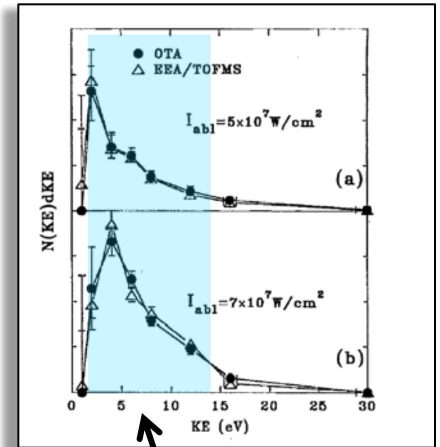
SIMION Simulations

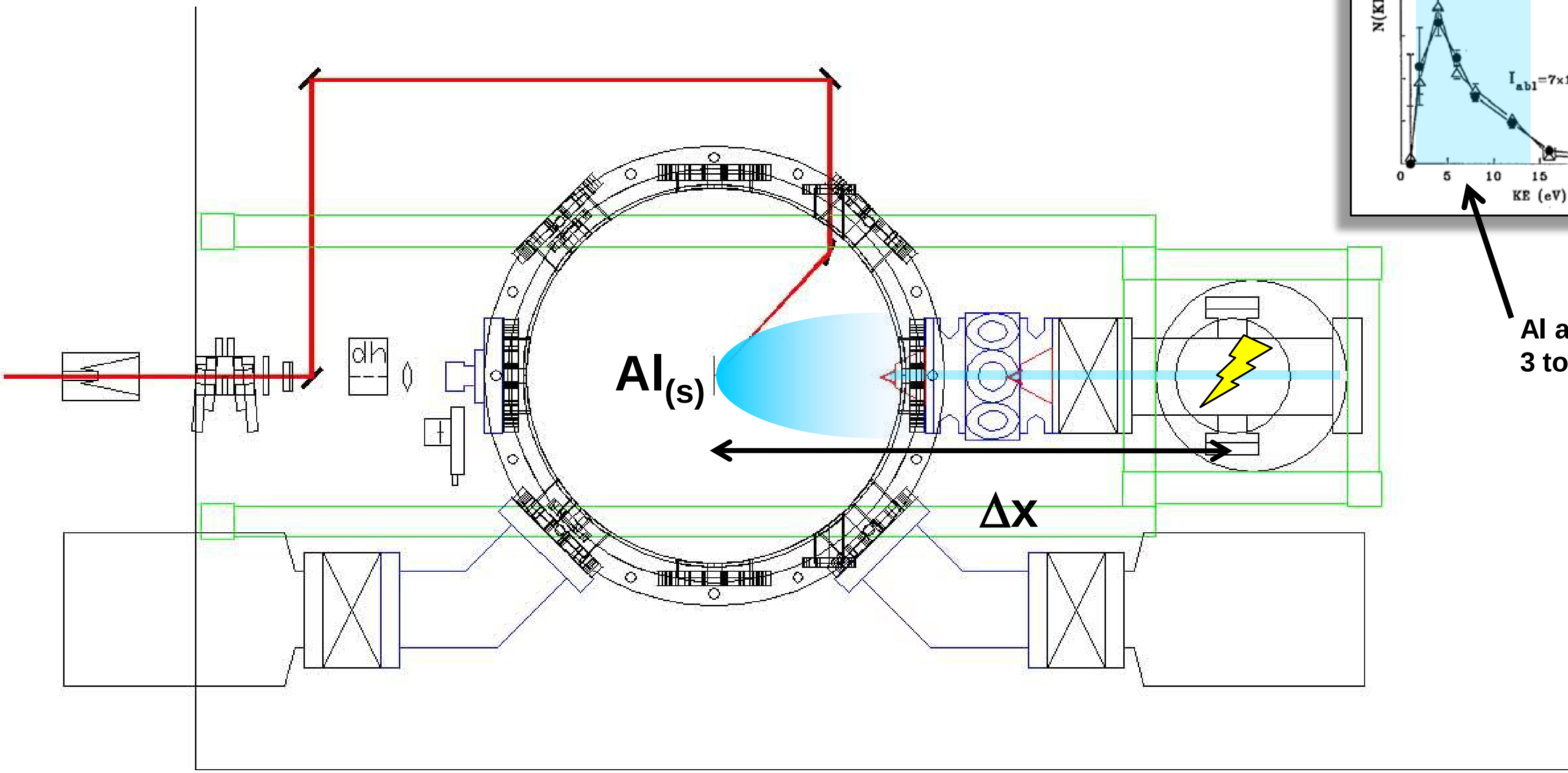


Aluminum Ablation Schematic

Use 1064 nm laser ablation of solid aluminum to produce fast (v ~ 10 km/s) Al atoms.

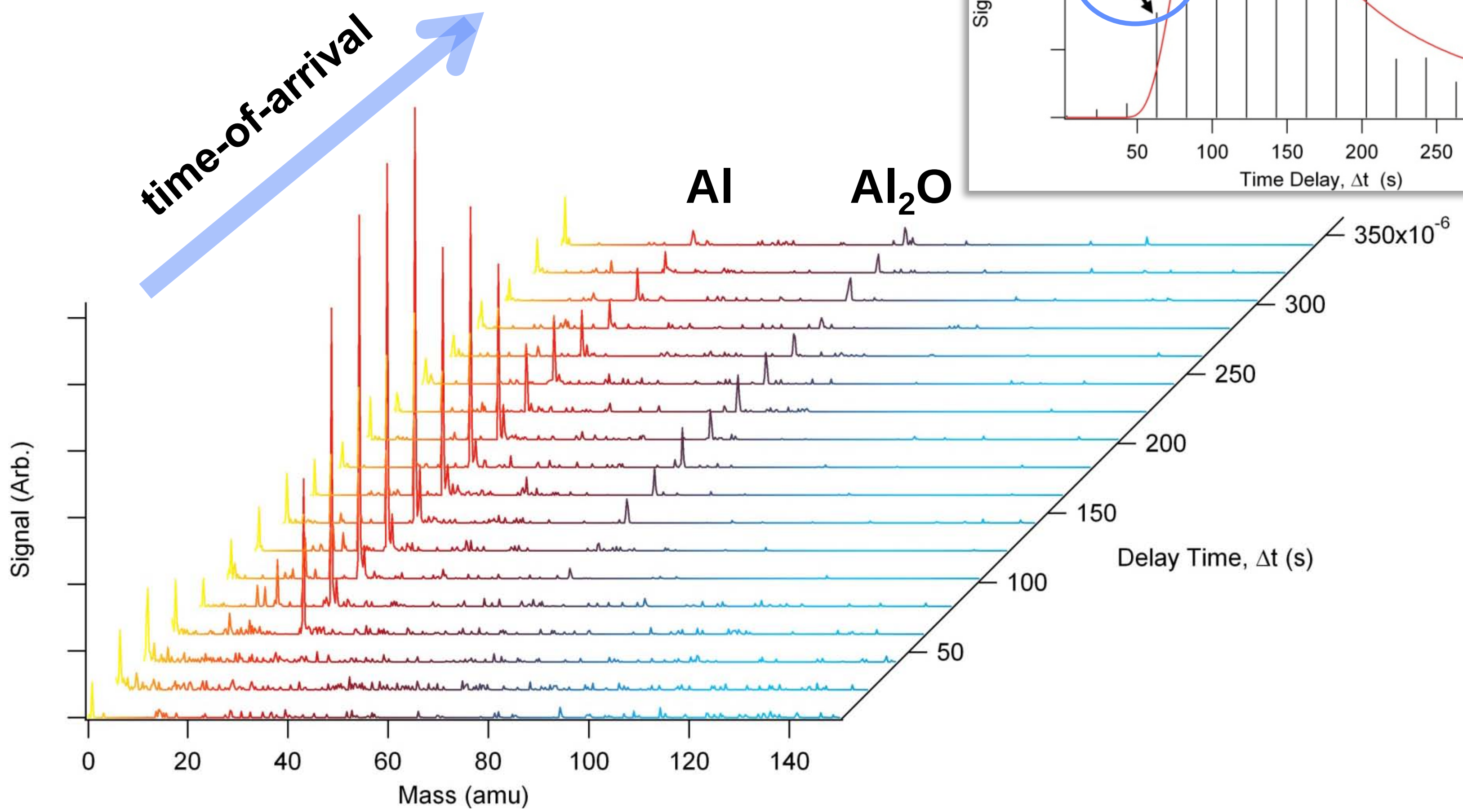
M. Macler, and M.E. Fajardo, Appl. Phys. Lett. **65**, 159 (1994).

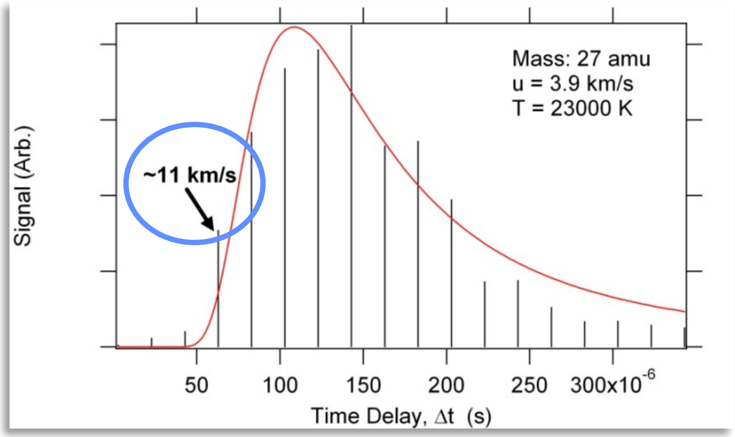




Al atom velocity 3 to 10 km/s

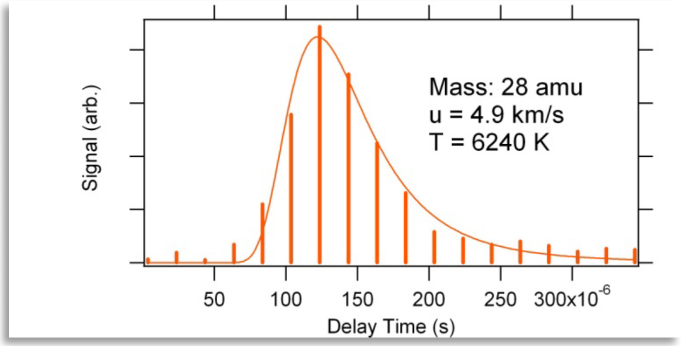
Aluminum Ablation Results

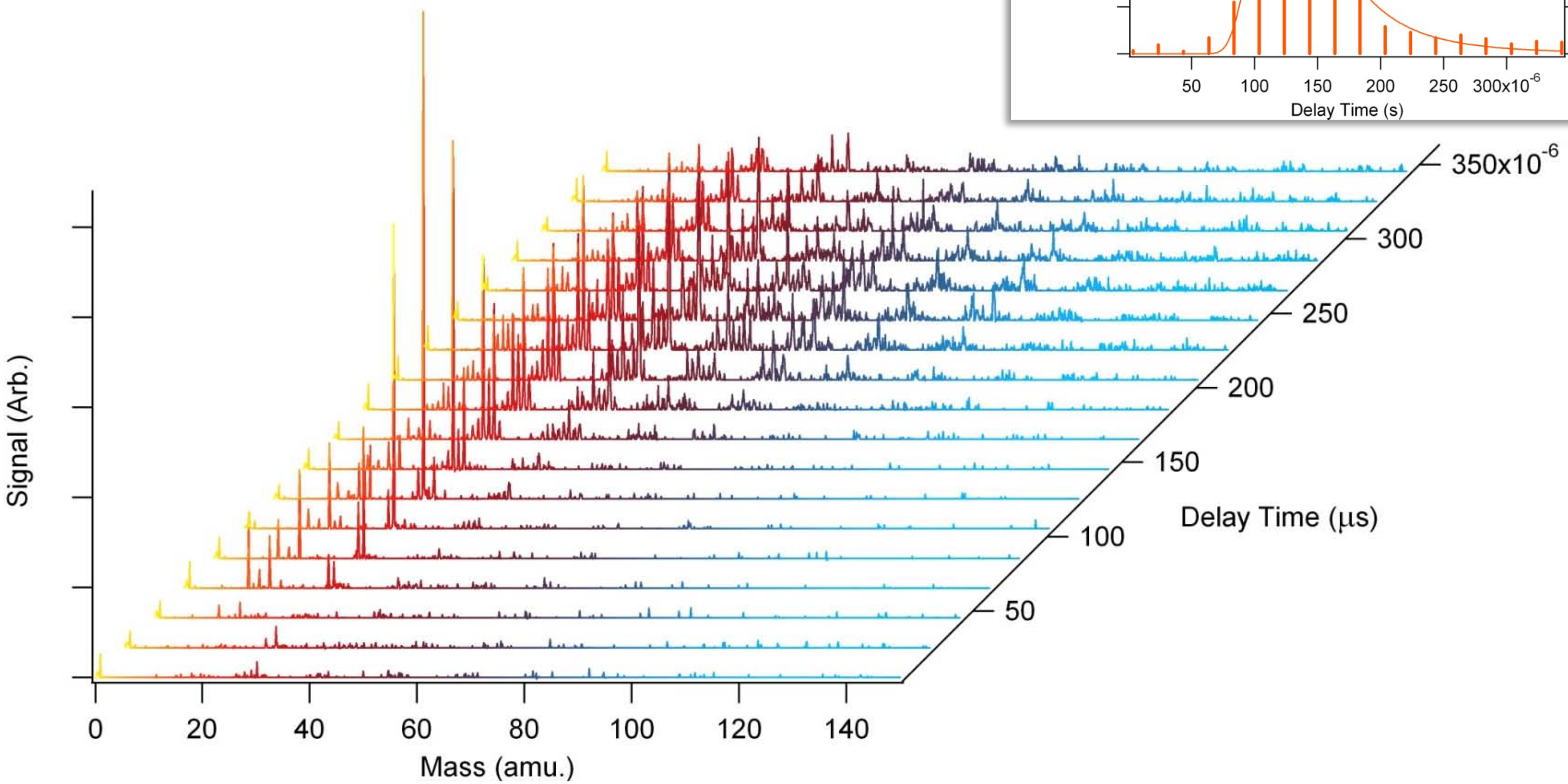




Nitrocellulose Laser Initiation

Fit m_{28} time-of-arrival data to Maxwell-Boltzman + u_{stream}





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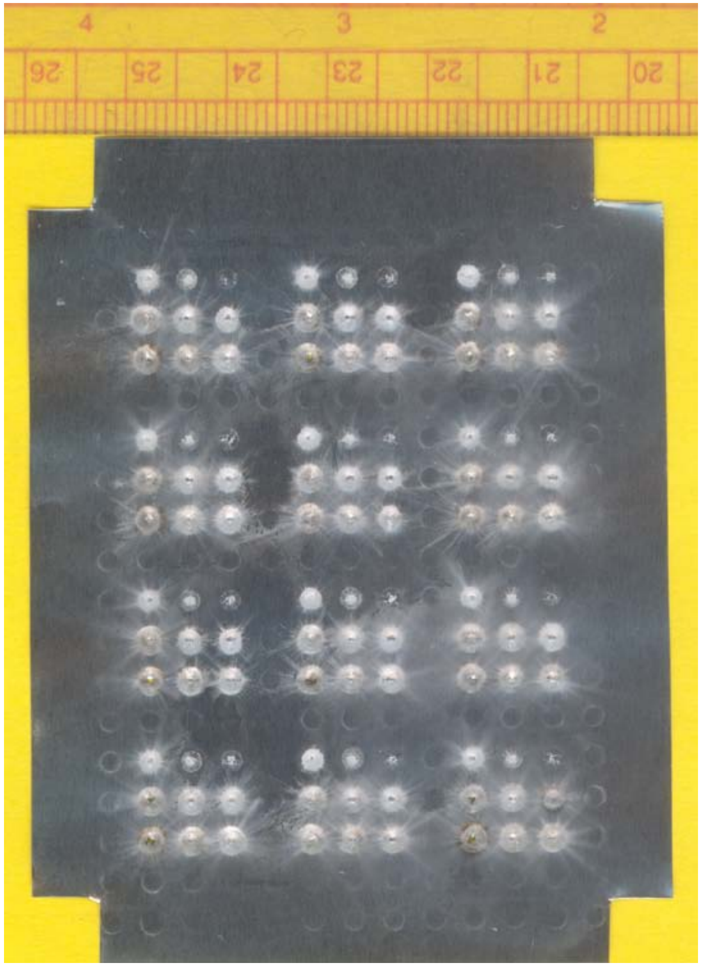
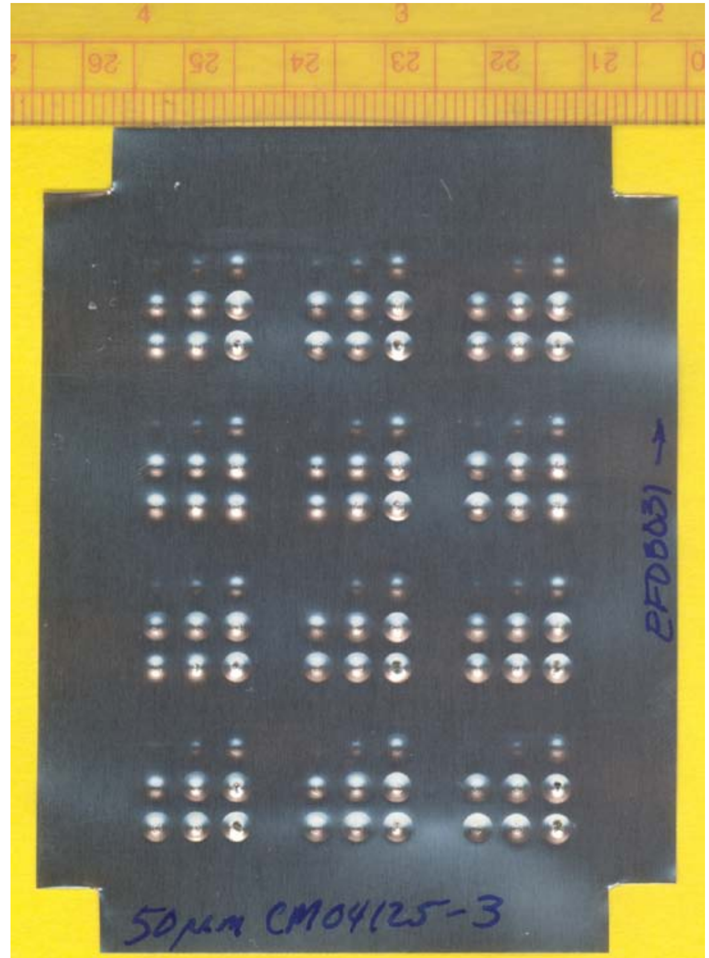
Conclusions

- Proposed a novel scheme for monitoring deflagration and “detonation-like” behaviors in small scale explosive samples-in-vacuum based on the chemical identities and velocity distributions of the gaseous products.
- Demonstrated detection of fast Al atoms (v ~ 10 km/s).
- Detected fast organic species from direct laser initiated nitrocellulose thin films.
- Determined semi-quantitative corrections for extracting neutral velocity distributions from measured time-of-arrival data.

Monday 12:15PM C2.00005
Benchtop Energetics:
Detection of Hyperthermal Species

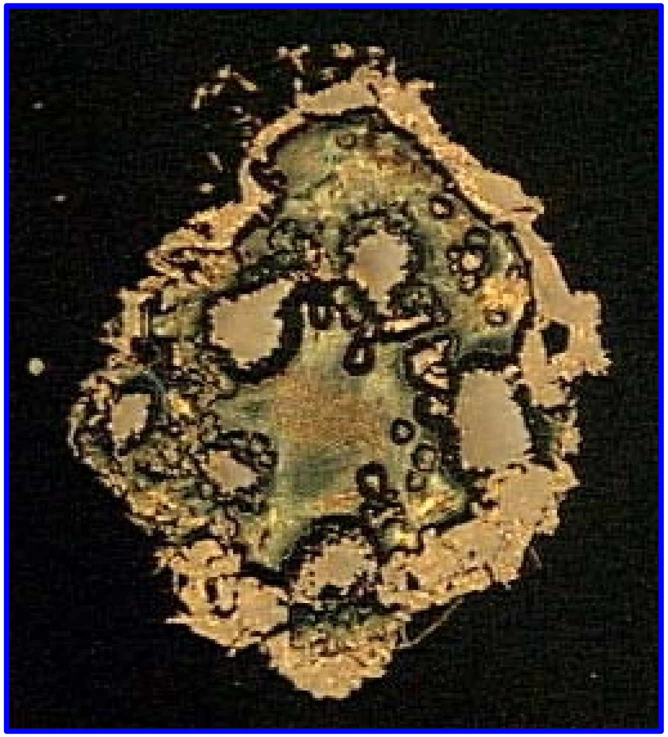
Future Directions – Laser Shocks

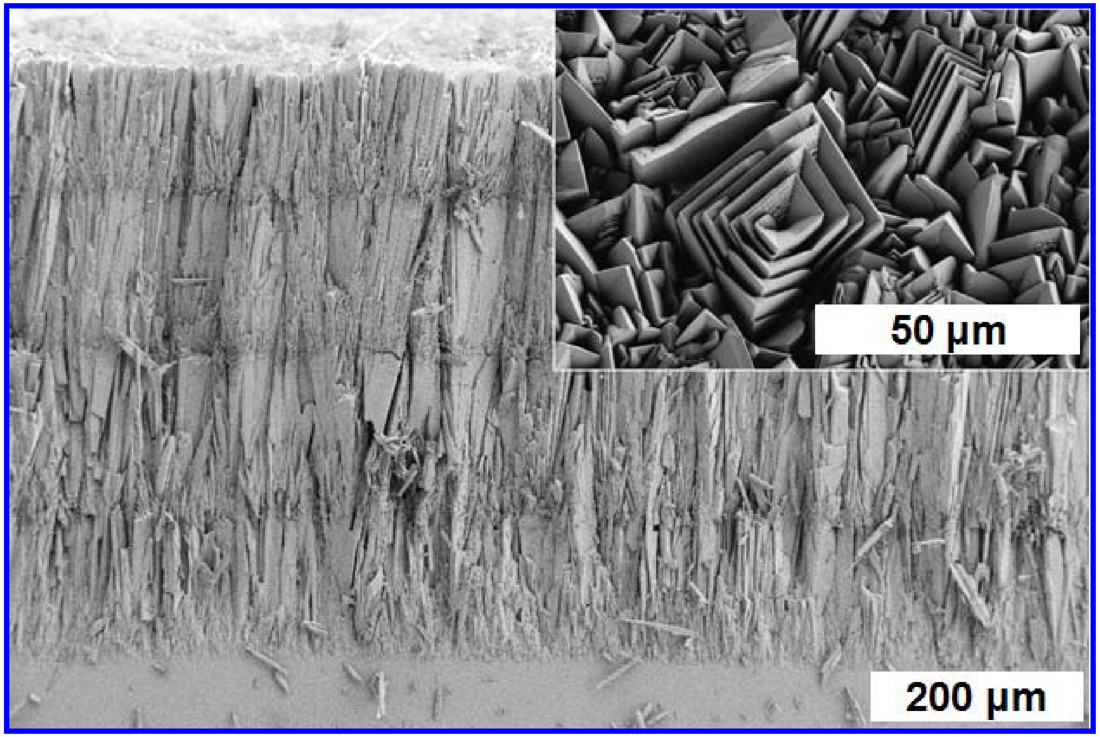




Wednesday 12:15PM M6.00006, Low-Order Modeling of Micro-Flier Impact with Thin Stationary Targets, MARK FRY & KEITH GONTHIER, Louisiana State University

Future Directions – Sample Prep.





drop-wise deposited PETN

physical vapor deposited PETN (Tappan)

Friday 11:00AM Z2.00001, Critical Detonation Thickness in Vapor-Deposited Penta-erythritol Tetranitrate (PETN) Films, ALEX TAPPAN, et al. Sandia National Labs

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